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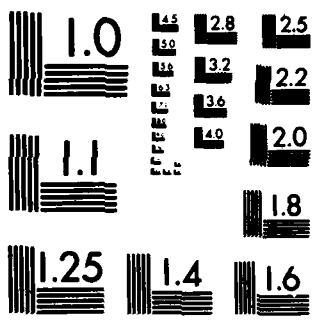

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Production of Short-Wavelength (XUV) Photons from Ion-Laser-Excited-Surface Charge Exchange: Li^{3+}, He^{+} + Si(111) Systems

by

Hai-Woong Lee and Thomas F. George

Prepared for Publication

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Department of Chemistry
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MODERATE LASER POWERS

20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Semiclassical calculations are carried out for the probabilities of electron transfer for Li^{3+} and He^{+} ions colliding with a Si(111) surface, where a laser is used to excite electrons in silicon from the valence band to surface states. It is shown that with a moderate-power laser, high inversion densities of Li^{2+} and He^{+} can be obtained, as necessary for high gain.

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PRODUCTION OF SHORT-WAVELENGTH (XUV) PHOTONS FROM ION-LASER-EXCITED-SURFACE CHARGE EXCHANGE: Li^{3+}, He^{+} + Si(111) SYSTEMS

Hai-Woong Lee

Department of Physics
Oakland University
Rochester, Michigan 48063

and

Thomas F. George

Department of Chemistry
University of Rochester
Rochester, New York 14627

A

ABSTRACT

Semiclassical calculations are carried out for the probabilities of electron transfer for Li^{3+} and He^{+} ions colliding with a Si(111) surface, where a laser is used to excite electrons in silicon from the valence band to surface states. It is shown that with a moderate-power laser, high inversion densities of Li^{2+} and He^{+} can be obtained, as necessary for high gain.

INTRODUCTION

It has been proposed[1,2] that some selected charge-exchange processes may serve as a means of achieving population inversion for short-wavelength (VUV and soft X-ray) lasers. In a recent study,[2,3] we have analyzed the possibility of obtaining coherent short-wavelength radiation based on neutralization of positive ions A^{m+} at a semiconductor surface S,

$$A^{m+} + S \rightarrow A^{(m-1)} + S^{+}. \qquad (1)$$

In particular, we have proposed that significant enhancement of gain can be achieved be electronically exciting the surface exposed to impinging ions. This is based on the observation that the capture probability is significantly higher for a surface electron (especially for an electron in normally unoccupied surface bands in the band gap region) than for a bulk electron.[2] If a large number of bulk electrons can be excited to surface bands by irradiating a surface with a source of appropriate power and wavelength, a significant enhancement of gain results. In Reference 3, cross-section and gain calculations on the system

$$He^{2+} + Si(111) \rightarrow He^{+}(3\ell) + Si^{+} \tag{2}$$

have been carried out.

Here we consider the following two processes:

$$Li^{3+} + Si(111) \rightarrow Li^{2+}(4\ell) + Si^{+}, \tag{3}$$

$$He^{+} + Si(111) \rightarrow He(2^{3}S) + Si^{+}. \tag{4}$$

Process (3) produces Li^{2+} predominantly in the third excited level, $Li^{2+}(4\ell)$. Process (4) is not a short-wavelength laser candidate, but it may represent an efficient way of producing metastable helium atoms, $He(2^{3}S)$.

CALCULATIONS AND RESULTS

The probability P for capture of a surface electron by the incoming ion (Li^{3+} or He^{+}) is calculated using the semiclassical formula[2,3]

$$P = 1 - \exp[-\frac{4}{v}\int_{0}^{\infty} dz\, \Gamma(z)], \tag{5}$$

where

$$\Gamma(z) = \frac{\pi}{\hbar}\rho(E_{o})\,|H_{IF}^{E_{o}}(z)|^{2}, \tag{6}$$

z is the ion-surface separation, v is the ion velocity assumed to be constant, ρ denotes the density of surface states, E_o is the resonance energy, and $H_{IF}^{E_o}$ is the coupling matrix element for an electron of energy E_o. [The transfer of a surface electron of energy E_o to the ion is an energy conserving process. Note that E_o changes with time because the initial and final potential energy curves vary with z.] We assume that charge exchange occurs mainly as a result of a repulsive force between the ion and the surface, and evaluate the coupling matrix element according to the formula

$$H_{IF}^{E_o}(z) = \frac{1}{2}|E_o + E_A|F(z). \qquad (7)$$

F is the overlap between the initial state (i.e., surface state) and the final state (i.e., atomic state into which the electron is captured) of the electron, and E_A is the effective ionization energy of the final state [$E_A \cong -7.6$ eV for $Li^{2+}(4\ell)$ and $E_A \cong -4.8$ eV for $He(2^3S)$, measured from the ionization level]. The resonance energy E_o is calculated by assuming that the potential energy curves are determined mainly by image forces, which yields

$$E_o = E_A + \frac{N(K-1)e^2}{4(K+1)z}, \qquad (8)$$

where N = 5 for Li^{3+}-Si and N = 1 for He^+-Si, and K is the dielectric constant of the solid (K = 11.8 for silicon). The density of surface states of silicon is taken to be[4] ρ/area = $4 \times 10^{14}/eV\cdot cm^2$. The integration in Equation (5) can now be performed numerically.

For Process (3) we obtain $P \cong 1 - \exp(-0.00645/v)$, where the velocity v is to be expressed in atomic units. At v = 0.1 a.u. $\cong 2.2 \times 10^7$ cm/sec we have $P \cong 0.063$, which yields the charge-exchange cross section $\sigma \cong 2.7$ Å^2. [The cross section σ was estimated using a simple formula $\sigma \cong \pi z_o^2 P$, where z_o is the ion-surface separation at which electron capture occurs. $z_o \cong 3.7 \sim 5.0$ Å for Process (3).] This value of cross section is large enough to give a high inversion density of Li^{2+} necessary for high gain, provided that high densities of Li^{3+} and surface electrons are provided. The required density of surface electrons[3] is typically on the order of $10^{16} \sim 10^{18}/cm^3$, which corresponds to the area density $10^9 - 10^{11}/cm^2$. This value of the area density of surface electrons appears to be well within the reach of a moderate-power infrared laser.[5]

For Process (2) we obtain $p \cong 1 - \exp(-0.0695/v)$, where the velocity v again is to be expressed in atomic units. At v = 0.1 a.u. $\cong 2.2 \times 10^7$cm/sec, we have $P \cong 0.50$, which yields $\sigma \cong 11$ Å^2 ($z_o \cong 2.6 \sim 4.5$ Å). For production of high-density metastable helium atoms one must pump a sufficient number of bulk electrons into surface bands. In view of the fact that this can be achieved with the use of a moderate-power laser, the density of metastable helium produced by the Process (2) may well be limited by the available density of He^+.

Finally, it should be mentioned that our analysis is based on a one-dimensional nearly-free-electron model of a surface[5,6] according to which a semiconductor has a direct gap. In reality, however, semiconductors like silicon have an indirect gap and the excitation of a surface by radiation may have to be accompanied by photon excitations.

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